

Coupling carbon oxidation and surface recession in Direct-simulation Monte Carlo code, SPARTA

V. Arias^{1,2,a)}, K. Swaminathan Gopalan³, A. Borner³, K. A. Stephani^{1,2}, and S. J. Plimpton⁴

¹ *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, 61801, USA*

² *Center for Hypersonics and Entry Systems Studies, University of Illinois at Urbana-Champaign, Urbana, IL, 61801, USA*

³ *Analytical Mechanics Associates Inc. at NASA Ames Research Center, Moffett Field, CA, 94045 USA*

⁴ *Sandia National Laboratories, Albuquerque, NM 87185, USA*

a) Corresponding author: arias6@illinois.edu

Ablative thermal protection system (TPS) materials for spacecraft are composites that are often made out of carbon-based reinforcement and a polymeric matrix. They endure high-temperature oxidation and surface recession when re-entering Earth's atmosphere. Ablation is the result of many coupled and competing thermal, mechanical, and chemical phenomena, and it is difficult to isolate the role of each on the overall degradation of the TPS. Here we develop an ablation model for material recession coupled explicitly to finite rate carbon oxidation in complex microstructures.

In this work, Stochastic PARallel Rarified-gas Time-accurate Analyzer (SPARTA) [1], a direct-simulation Monte Carlo (DSMC) code, is modified to allow oxidation-driven ablation of implicitly defined carbon surfaces. In SPARTA, implicit surfaces are generated from the grid corner point values via a marching cubes algorithm, therefore creating a new set of surface elements every time ablation is performed. The finite-rate oxidation model developed by Gopalan et. al [2], was adapted to tally surface reactions and other surface data on a per-grid cell basis. The ablation functionality was also adjusted so once the reactions have occurred, the number of reactions leading to CO formation can be converted to corner point reduction values; therefore, carbon removal is directly proportional to surface recession. We also develop robust algorithms which handle the evolution of the flow cells and solid material regions, including split cells (flow cell divided in two by a solid surface). Finally, we demonstrate our implicit chemistry model for 2D and 3D geometries by producing reaction statistics and detailed visualization of oxidation-induced material recession at the microscale.

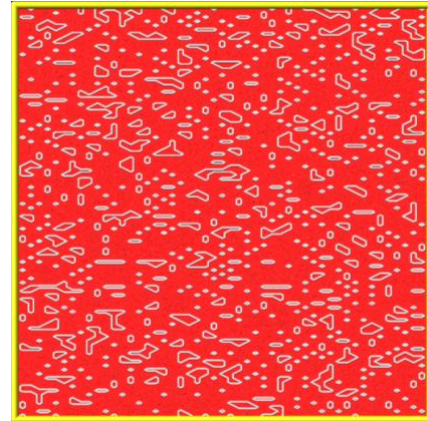


Fig. 1. 2d flow through random porous media, where surface line segments are in white

ACKNOWLEDGEMENTS

This work was supported through a NASA Space Technology Graduate Research Opportunities (NSTGRO) Fellowship (Grant 80NSSC20K1211, Technical Sponsor Dr. Justin Haskins).

REFERENCES

- [1] Plimpton, S. J., et al. "Direct simulation Monte Carlo on petaflop supercomputers and beyond." *Physics of Fluids* 31.8 (2019): 086101.
- [2] Swaminathan-Gopalan, Krishnan, et al. "Development and validation of a finite-rate model for carbon oxidation by atomic oxygen." *Carbon* 137 (2018): 313-332.